

FULL SEARCH INITIATED 14:18:46 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 3542 TO ITERATE

100.0% PROCESSED 3542 ITERATIONS 150 ANSWERS  
 SEARCH TIME: 00.00.01

L3 150 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

156.26

156.47

FILE 'HCAPLUS' ENTERED AT 14:18:52 ON 31 MAR 2004  
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FILE COVERS 1907 - 31 Mar 2004 VOL 140 ISS 14  
 FILE LAST UPDATED: 30 Mar 2004 (20040330/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 28 L3

=> s 14 and yu, k?/au

2573 YU, K?/AU

L5 2 L4 AND YU, K?/AU

=> d 15, ibib abs fhitstr, 1-2

L5 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER:	2003:511082 HCAPLUS
DOCUMENT NUMBER:	139:85343
TITLE:	Preparation of 2-(heterocyclylmethyl)benzimidazoles as respiratory syncytial virus antiviral agents
INVENTOR(S):	Yu, Kuo-long; Wang, Xiangdong; Sun, Yaxiong; Cianci, Christopher; Thuring, Jan Willem; Combrink, Keith; Meanwell, Nicholas; Zhang, Yi; Civiello, Rita L.
PATENT ASSIGNEE(S):	Bristol-Myers Squibb Company, USA
SOURCE:	PCT Int. Appl., 149 pp.
	CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

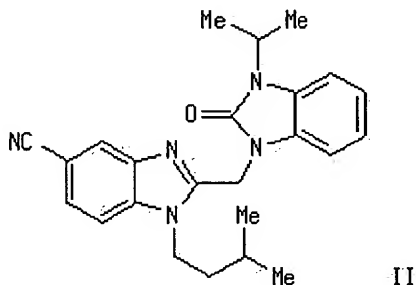
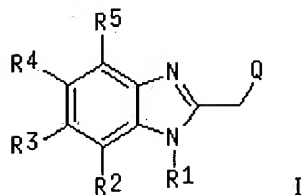
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2003053344</u>	A2	20030703	<u>WO 2002-US39220</u>	20021206
<u>WO 2003053344</u>	A3	20031113		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

<u>US 2003207868</u>	A1	20031106	<u>US 2002-309505</u>	20021204
<u>PRIORITY APPLN. INFO.:</u>			<u>US 2001-339025P</u>	P 20011210
<u>OTHER SOURCE(S):</u>			MARPAT 139:85343	

GI



AB Title compds. I [wherein R1 = (CRaRb)nX; R2 = H; R3 = CONRhRi, CO2Rd, or (un)substituted alkyl; R4 = NH2, CONRhRi, heteroaryl, alkenyl, CO2Rd, N=CPh2, C(NOHNH2, C(NH)NH2, or (un)substituted alkyl; R5 = CO2Rj or (un)substituted alkyl or alkenyl; Q = (un)substituted benzimidazolyl, benzotriazolyl, imidazopyridinyl, quinolinyl, quinazolinyl, benzyloxy, etc.; X = H or (un)substituted alkyl; Ra and Rb = independently H or (halo)alkyl; Rd = alkyl; Rh and Ri = independently H or alkyl; Rj = H or alkyl; n = 1-6; and pharmaceutically acceptable salts thereof] were prepd. as antiviral compds. More particularly, the invention provides 2-(heterocyclylmethyl)benzimidazole derivs. for the treatment of respiratory syncytial virus (RSV) infection. For example, 1-isopropyl-1,3-dihydrobenzimidazol-2-one was coupled with 2-chloromethyl-1-(3-methylbutyl)-1H-benzimidazole-5-carbonitrile in the presence of Cs2CO3 in DMF to give II (95%). Disclosed compds. protected HEP-2 cells from RSV-induced cytopathic effects with EC50 values between 50  $\mu$ M and 0.001  $\mu$ M, compared to an EC50 of 3  $\mu$ M for ribavirin. I also displayed antiviral activity by reducing viral protein expression in HEP-2 cells with EC50 values between 50  $\mu$ M and 0.001  $\mu$ M, compared to an EC50 value of 3  $\mu$ M for ribavirin. Thus, I and compns. comprising I are useful for the treatment of RSV infections.

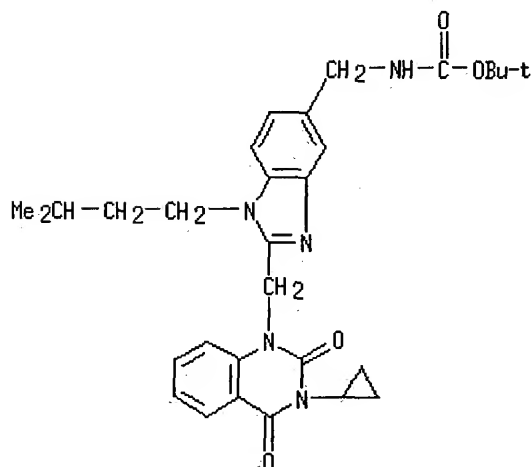
IT 554458-05-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(antiviral agent; prepn. of (heterocyclylmethyl)benzimidazoles as RSV antiviral agents)

RN 554458-05-8 HCAPLUS

CN Carbamic acid, [[2-[(3-cyclopropyl-3,4-dihydro-2,4-dioxo-1(2H)-quinazolinyl)methyl]-1-(3-methylbutyl)-1H-benzimidazol-5-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2002:556140 HCAPLUS  
DOCUMENT NUMBER: 137:125159  
TITLE: Preparation and antiviral activity of heterocyclic substituted 2-methylbenzimidazole antiviral agents  
INVENTOR(S): Yu, Kuo-Long; Civiello, Rita L.; Combrink, Keith D.; Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong; Meanwell, Nicholas; Venables, Brian Lee; Zhang, Yi; Pearce, Bradley C.; Yin, Zhiwei; Thuring, Jan Willem  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 89 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002099208	A1	20020725	US 2001-994012	20011116
WO 2002062290	A2	20020815	WO 2001-US45149	20011120
WO 2002062290	A3	20021121		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1343499 A2 20030917 EP 2001-270116 20011120

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.:

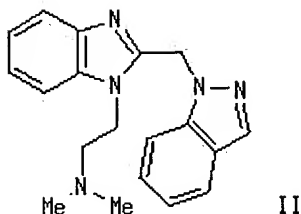
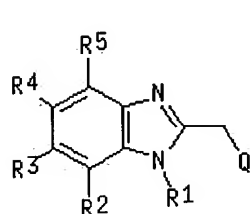
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WO 2001-US45149 W 20011120

OTHER SOURCE(S):

MARPAT 137:125159

GI



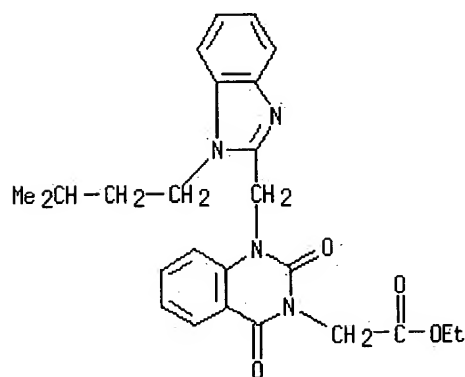
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IT 443987-05-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. and use of heterocyclic substituted 2-methyl-benzimidazole antiviral agents)

RN 443987-05-1 HCAPLUS

CN 3(2H)-Quinazolineacetic acid, 1,4-dihydro-1-[[1-(3-methylbutyl)-1H-benzimidazol-2-yl]methyl]-2,4-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 14:16:55 ON 31 MAR 2004)

FILE 'REGISTRY' ENTERED AT 14:17:09 ON 31 MAR 2004

L1 STRUCTURE UPLOADED

L2 5 S L1  
L3 150 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:18:52 ON 31 MAR 2004

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L5 2 S L4 AND YU, K?/AU

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L6 26 L4 NOT L5

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12 CIVIELLO, R?/AU  
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L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER:	2002:556140 HCAPLUS
DOCUMENT NUMBER:	137:125159
TITLE:	Preparation and antiviral activity of heterocyclic substituted 2-methylbenzimidazole antiviral agents

INVENTOR(S): Yu, Kuo-Long; Civiello, Rita L.; Combrink, Keith D.;  
 Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong;  
 Meanwell, Nicholas; **Venables, Brian Lee**; Zhang, Yi;  
 Pearce, Bradley C.; Yin, Zhiwei; Thuring, Jan Willem

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 89 pp.  
 CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002099208	A1	20020725	US 2001-994012	20011116
WO 2002062290	A2	20020815	WO 2001-US45149	20011120
WO 2002062290	A3	20021121		

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 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,  
 PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,  
 UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,  
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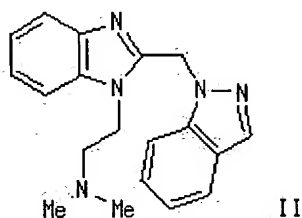
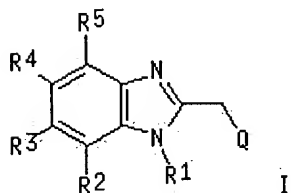
EP 1343499 A2 20030917 EP 2001-270116 20011120

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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.: US 2000-257139P P 20001220  
 WO 2001-US45149 W 20011120

OTHER SOURCE(S): MARPAT 137:125159

GI



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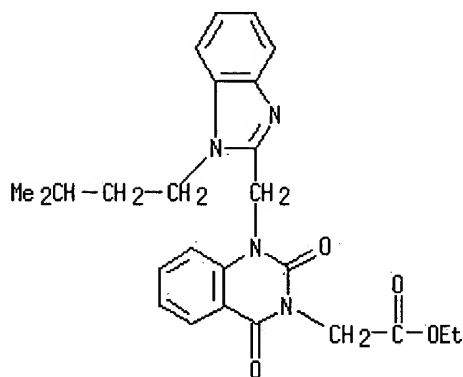
IT **443987-05-1P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP  
(Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. and use of heterocyclic substituted 2-methyl-benzimidazole  
antiviral agents)

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benzimidazol-2-yl]methyl]-2,4-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



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L2 5 S L1

L3 150 S L1 FULL

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L5 2 S L4 AND YU, K?/AU

L6 26 S L4 NOT L5

L7 0 S L6 AND CIVIELLO, R?/AU

L8 2 S L4 AND COMBRINK, K?/AU

L9 0 S L8 NOT L5

L10 1 S L4 AND SIN, N?/AU

L11 0 S L10 NOT L8

L12 2 S L4 AND WANG, X?/AU

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L20 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing  
 Text References

ACCESSION NUMBER: 2002:556140 HCAPLUS  
 DOCUMENT NUMBER: 137:125159  
 TITLE: Preparation and antiviral activity of heterocyclic substituted 2-methylbenzimidazole antiviral agents  
 INVENTOR(S): Yu, Kuo-Long; Civiello, Rita L.; Combrink, Keith D.; Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong; Meanwell, Nicholas; Venables, Brian Lee; Zhang, Yi; Pearce, Bradley C.; Yin, Zhiwei; Thuring, Jan Willem  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 89 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

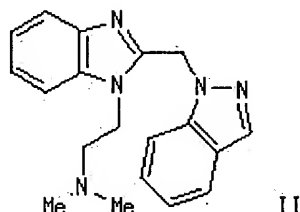
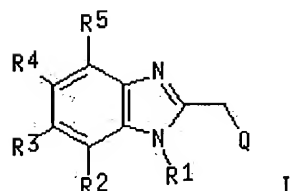
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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PRIORITY APPLN. INFO.: US 2000-257139P P 20001220  
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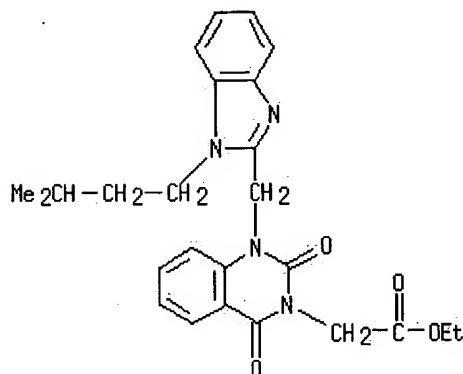
(un)substituted alkyl; X = H, C1-6 (un)substituted alkyl; n = 1-6; R2, R5 = independently H or halogen; R3, R4 = independently H, halogen, C1-6 (un)substituted alkyl; Q = heterocyclic group], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a four-step synthesis of II, starting with 2-(chloromethyl)benzimidazole, was given. The antiviral activity of these compds. against respiratory syncytial virus (RSV) was detd. in HEP-2 (ATCC CCL 23) cells. The title compds. I, disclosed herein, show antiviral activity with EC50s between 50  $\mu$ M and 0.001  $\mu$ M.

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L13 0 S L12 NOT L8

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L15 0 S L14 NOT L8

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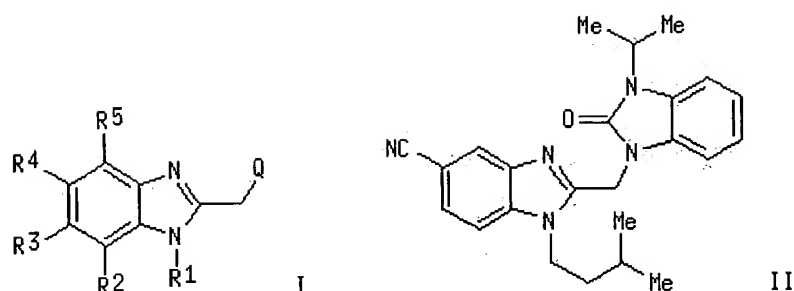
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L21 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

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DOCUMENT NUMBER:	139:85343
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PATENT ASSIGNEE(S):	Bristol-Myers Squibb Company, USA
SOURCE:	PCT Int. Appl., 149 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
<u>PATENT INFORMATION:</u>	

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WO 2003053344	A2	20030703	WO 2002-US39220	20021206
WO 2003053344	A3	20031113		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003207868	A1	20031106	US 2002-309505	20021204
PRIORITY APPLN. INFO.:		US 2001-339025P P 20011210		
OTHER SOURCE(S):		MARPAT 139:85343		
GI				



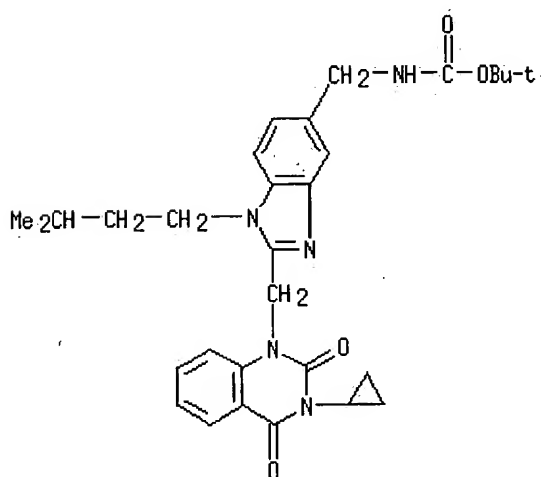
AB Title compds. I [wherein R1 = (CRaRb)<sub>n</sub>X; R2 = H; R3 = CONRhRi, CO2Rd, or (un)substituted alkyl; R4 = NH2, CONRhRi, heteroaryl, alkenyl, CO2Rd, N=CPh2, C(NOH)NH2, C(NH)NH2, or (un)substituted alkyl; R5 = CO2Rj or (un)substituted alkyl or alkenyl; Q = (un)substituted benzimidazolyl, benzotriazolyl, imidazopyridinyl, quinolinyl, quinazolinyl, benzyloxy, etc.; X = H or (un)substituted alkyl; Ra and Rb = independently H or (halo)alkyl; Rd = alkyl; Rh and Ri = independently H or alkyl; Rj = H or alkyl; n = 1-6; and pharmaceutically acceptable salts thereof] were prepd. as antiviral compds. More particularly, the invention provides 2-(heterocyclylmethyl)benzimidazole derivs. for the treatment of respiratory syncytial virus (RSV) infection. For example, 1-isopropyl-1,3-dihydrobenzimidazol-2-one was coupled with 2-chloromethyl-1-(3-methylbutyl)-1H-benzimidazole-5-carbonitrile in the presence of Cs2CO3 in DMF to give II (95%). Disclosed compds. protected HEp-2 cells from RSV-induced cytopathic effects with EC50 values between 50  $\mu$ M and 0.001  $\mu$ M, compared to an EC50 of 3  $\mu$ M for ribavirin. I also displayed antiviral activity by reducing viral protein expression in HEp-2 cells with EC50 values between 50  $\mu$ M and 0.001  $\mu$ M, compared to an EC50 value of 3  $\mu$ M for ribavirin. Thus, I and compns. comprising I are useful for the treatment of RSV infections.

IT 554458-05-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(antiviral agent; prepn. of (heterocyclylmethyl)benzimidazoles as RSV antiviral agents)

RN 554458-05-8 HCAPLUS

CN Carbamic acid, [[2-[(3-cyclopropyl-3,4-dihydro-2,4-dioxo-1(2H)-quinazolinyl)methyl]-1-(3-methylbutyl)-1H-benzimidazol-5-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L21 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

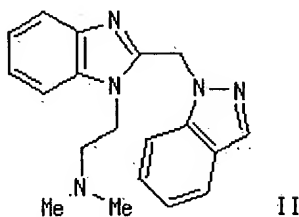
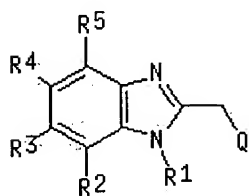
Full Text	Citing References
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ACCESSION NUMBER: 2002:556140 HCAPLUS  
DOCUMENT NUMBER: 137:125159  
TITLE: Preparation and antiviral activity of heterocyclic substituted 2-methylbenzimidazole antiviral agents  
INVENTOR(S): Yu, Kuo-Long; Civiello, Rita L.; Combrink, Keith D.; Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong; Meanwell, Nicholas; Venables, Brian Lee; Zhang, Yi; Pearce, Bradley C.; Yin, Zhiwei; Thuring, Jan Willem  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 89 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002099208	A1	20020725	US 2001-994012	20011116
WO 2002062290	A2	20020815	WO 2001-US45149	20011120
WO 2002062290	A3	20021121		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1343499	A2	20030917	EP 2001-270116	20011120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.: US 2000-257139P P 20001220  
WO 2001-US45149 W 20011120

OTHER SOURCE(S): MARPAT 137:125159  
GI



AB The title compds. [I; R1 = (CRaRb)<sub>n</sub>X; Ra, Rb = independently H, C1-6 (un)substituted alkyl; X = H, C1-6 (un)substituted alkyl; n = 1-6; R2, R5 = independently H or halogen; R3, R4 = independently H, halogen, C1-6 (un)substituted alkyl; Q = heterocyclic group], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a four-step synthesis of II, starting with 2-(chloromethyl)benzimidazole, was given. The antiviral activity of these compds. against respiratory syncytial virus (RSV) was

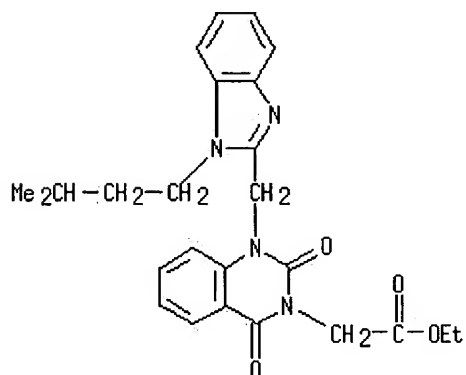
detd. in HEp-2 (ATCC CCL 23) cells. The title compds. I, disclosed herein, show antiviral activity with EC50s between 50  $\mu$ M and 0.001  $\mu$ M.

IT **443987-05-1P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. and use of heterocyclic substituted 2-methyl-benzimidazole antiviral agents)

RN **443987-05-1** HCAPLUS

CN 3(2H)-Quinazolineacetic acid, 1,4-dihydro-1-[[1-(3-methylbutyl)-1H-benzimidazol-2-yl]methyl]-2,4-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	45.06	201.53
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.16	-4.16

FILE 'CAOLD' ENTERED AT 14:23:17 ON 31 MAR 2004

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 14:16:55 ON 31 MAR 2004)

FILE 'REGISTRY' ENTERED AT 14:17:09 ON 31 MAR 2004

L1 STRUCTURE UPLOADED

L2 5 S L1

L3 150 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:18:52 ON 31 MAR 2004

L4 28 S L3

L5 2 S L4 AND YU, K?/AU

L6 26 S L4 NOT L5

L7 0 S L6 AND CIVIELLO, R?/AU

L8 2 S L4 AND COMBRINK, K?/AU

L9 0 S L8 NOT L5

L10 1 S L4 AND SIN, N?/AU

L11 0 S L10 NOT L8

L12 2 S L4 AND WANG, X?/AU

L13 0 S L12 NOT L8

L14 2 S L4 AND MEANWELL, N?/AU

L15 0 S L14 NOT L8

L16 1 S L4 AND VENABLES, B?/AU

L17 2 S L4 AND ZHANG, Y?/AU

L18 0 S L17 NOT L5

L19 0 S L4 AND PEARC, B?/AU

L20 1 S L4 AND YIN, Z?/AU

L21 2 S L4 AND THURING, J?/AU

FILE 'CAOLD' ENTERED AT 14:23:17 ON 31 MAR 2004

=> s 13

L22 1 L3

=> d 122, all, 1

L22 ANSWER 1 OF 1 CAOLD COPYRIGHT 2004 ACS on STN

AN CA52:13005d CAOLD

TI benzimidazoles as specific inhibitors of vitamin B12 or thymine in bacterial mutants

AU Scott, Dwight B. M.; Rogers, M. L.; Rose, C.

IT 53-82-7 585-95-5 3363-56-2 4887-80-3 4887-82-5 6478-73-5  
7479-04-1 10527-53-4 10597-49-6 10597-50-9 10597-51-0 10597-52-1  
10597-54-3 10597-55-4 15476-97-8 21087-77-4 23249-97-0 30411-81-5  
37724-28-0 50607-90-4 55299-95-1 82326-55-4 100958-72-3 101083-91-4  
101861-05-6 102169-82-4 109670-23-7

=> fil reg; d acc 109670-23-7; fil CAOLD

FILE 'REGISTRY' ENTERED AT 14:23:32 ON 31 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 109670-23-7 REGISTRY

CN Pyridinium, 1-[[1-(phenylmethyl)-1H-benzimidazol-2-yl]methyl]-, chloride (9CI) (CA INDEX NAME)

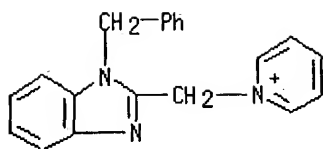
OTHER CA INDEX NAMES:

CN 1-(1-Benzyl-2-benzimidazolylmethyl)pyridinium chloride (6CI)

MF C20 H18 N3 . Cl

SR CAOLD

LC STN Files: CAOLD

# Cl<sup>-</sup>

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 14:23:32 ON 31 MAR 2004

=&gt; file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	205.18
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.16

FILE 'REGISTRY' ENTERED AT 14:23:37 ON 31 MAR 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 MAR 2004 HIGHEST RN 669048-54-8

DICTIONARY FILE UPDATES: 30 MAR 2004 HIGHEST RN 669048-54-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=&gt;

L23 STRUCTURE UPLOADED

=&gt; d 123

L23 HAS NO ANSWERS

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X 36 AK 37H 38

X 34 H 35

C 32 N 33

C 28 O 29 S 30 N 31

C 25 S 26 N 27  
Page 1-A

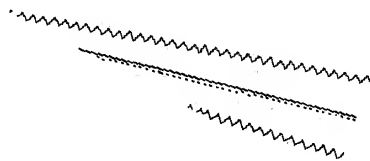
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Page 1-B

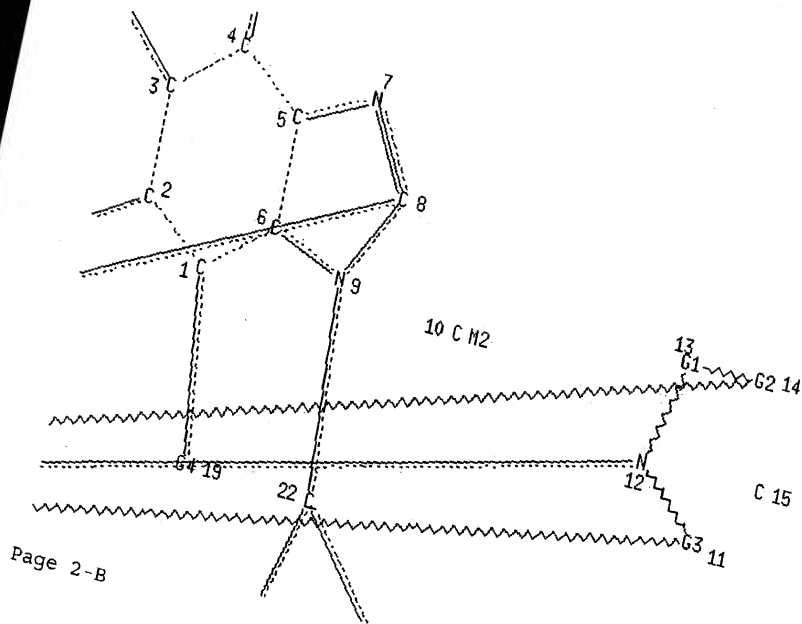
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21 G5

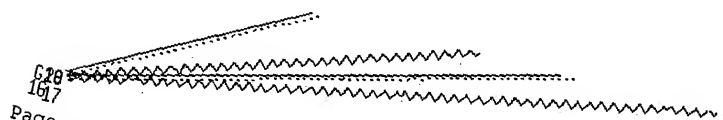
Page 2-A



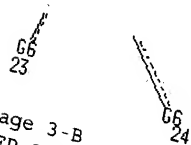




Page 2-B



Page 3-A



Page 3-B

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VAR G2=28/29/30/31  
VAR G3=32/33  
VAR G4=34/35  
VAR G5=36/37/38  
VAR G6=39/40

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 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 8  
 NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE

=> s 123

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 SAMPLE SCREEN SEARCH COMPLETED - 526 TO ITERATE

100.0% PROCESSED 526 ITERATIONS 50 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 9145 TO 11895  
 PROJECTED ANSWERS: 1147 TO 2253

L24 50 SEA SSS SAM L23

=> s 123 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:25:19 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 11076 TO ITERATE

100.0% PROCESSED 11076 ITERATIONS 1620 ANSWERS  
 SEARCH TIME: 00.00.01

L25 1620 SEA SSS FUL L23

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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FULL ESTIMATED COST	156.26	361.44
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	0.00	-4.16

FILE 'HCAPLUS' ENTERED AT 14:25:26 ON 31 MAR 2004  
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FILE COVERS 1907 - 31 Mar 2004 VOL 140 ISS 14  
 FILE LAST UPDATED: 30 Mar 2004 (20040330/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L26 212 L25

=> s 126 and civiello, r?/au

12 CIVIELLO, R?/AU

L27 6 L26 AND CIVIELLO, R?/AU

=> d his

(FILE 'HOME' ENTERED AT 14:16:55 ON 31 MAR 2004)

FILE 'REGISTRY' ENTERED AT 14:17:09 ON 31 MAR 2004

L1 STRUCTURE UPLOADED

L2 5 S L1

L3 150 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:18:52 ON 31 MAR 2004

L4 28 S L3

L5 2 S L4 AND YU, K?/AU

L6 26 S L4 NOT L5

L7 0 S L6 AND CIVIELLO, R?/AU

L8 2 S L4 AND COMBRINK, K?/AU

L9 0 S L8 NOT L5

L10 1 S L4 AND SIN, N?/AU

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L15 0 S L14 NOT L8

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L18 0 S L17 NOT L5

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L20 1 S L4 AND YIN, Z?/AU

L21 2 S L4 AND THURING, J?/AU

FILE 'CAOLD' ENTERED AT 14:23:17 ON 31 MAR 2004

L22 1 S L3

FILE 'REGISTRY' ENTERED AT 14:23:32 ON 31 MAR 2004

FILE 'CAOLD' ENTERED AT 14:23:32 ON 31 MAR 2004

FILE 'REGISTRY' ENTERED AT 14:23:37 ON 31 MAR 2004

L23 STRUCTURE UPLOADED

L24 50 S L23

L25 1620 S L23 FULL

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L26 212 S L25

L27 6 S L26 AND CIVIELLO, R?/AU

=> s l27 not l5

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=> s l28 not l8

L29 4 L28 NOT L8

=> s l29 not l10

L30 4 L29 NOT L10

=> s l30 not l12

L31 4 L30 NOT L12

=> s l30 not l14

L32 4 L30 NOT L14

=> l 30 not l16

L IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter  
"HELP COMMANDS" at an arrow prompt (=>).

=> s l30 not l16

L33 4 L30 NOT L16

=> s l30 not l17

L34 4 L30 NOT L17

=> s l33 not l20

L35 4 L33 NOT L20

=> s l33 not l21

L36 4 L33 NOT L21

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L33 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2003:442751 HCAPLUS

DOCUMENT NUMBER: 139:159456

TITLE: Fundamental structure-activity relationships  
associated with a new structural class of respiratory  
syncytial virus inhibitor

AUTHOR(S): Yu, Kuo-Long; Zhang, Yi; Civiello, Rita L.; Kadow,  
Kathleen F.; Cianci, Christopher; Krystal, Mark;  
Meanwell, Nicholas A.

CORPORATE SOURCE: Department of Chemistry, The Bristol-Myers Squibb

Pharmaceutical Research Institute, Wallingford, CT,  
06492, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003),  
13(13), 2141-2144  
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

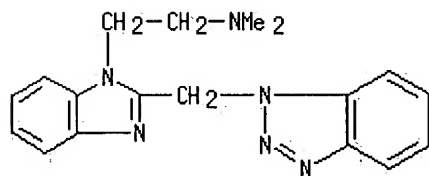
OTHER SOURCE(S): CASREACT 139:159456

AB Structure-activity relationships surrounding the dialkylamino side chain  
of a series of benzotriazole-derived inhibitors of respiratory syncytial  
virus fusion were examd. The results indicate that the topol. of the side  
chain is important but the terminus element offers considerable latitude  
to modulate phys. properties.

IT 5823-60-9  
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic  
use); BIOL (Biological study); USES (Uses)  
(fundamental structure-activity relationships assocd. with a new  
structural class of respiratory syncytial virus inhibitor)

RN 5823-60-9 HCAPLUS

CN 1H-Benzimidazole-1-ethanamine, 2-(1H-benzotriazol-1-ylmethyl)-N,N-dimethyl-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2002:256041 HCAPLUS

DOCUMENT NUMBER: 136:294826

TITLE: Preparation of benzimidazolone antiviral agents

INVENTOR(S): Yu, Kuo-Long; Civiello, Rita; Combrink, Keith;  
Gulgeze, Hatice Belgin; Pearce, Bradley C.; Wang,  
Xiangdong; Meanwell, Nicholas A.; Zhang, Yi

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 216 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002026228	A1	20020404	WO 2001-US29493	20010927
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
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US 6506738

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US 2001-952736

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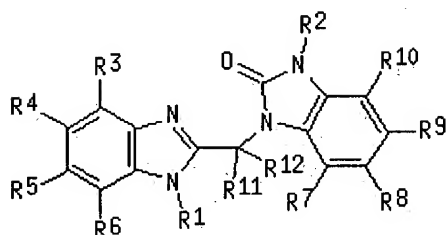
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US 2000-235804P P 20000927

OTHER SOURCE(S):

MARPAT 136:294826

GI



I

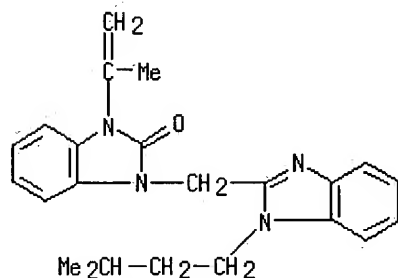
AB The title compds. [I; R1 = (CRvRw)nX; Rv, Rw = H, (halo)alkyl, (halo)alkenyl; X = H, (un)substituted alkyl, alkenyl; n = 1-6; R2 = H, alkyl, Ph, etc.; R3, R6, R7, R10 = H; R5, R8, R9 = H, halo, CF3; R4 = H, halo, CN, etc.; R11, R12 = H], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a 4-step synthesis of I [R1 = CH2CH2CHMe2; R2 = C(:CH2)Me; R3-R12 = H], starting with 2-(chloromethyl)benzimidazole, was given. The title compds. I showed antiviral activity against RSV with EC50's between 50  $\mu$ M and 0.001  $\mu$ M.

IT 406940-52-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of benzimidazolone antiviral agents)

RN 406940-52-1 HCAPLUS

CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-[[1-(3-methylbutyl)-1H-benzimidazol-2-yl]methyl]-3-(1-methylethenyl)- (9CI) (CA INDEX NAME)



NO

REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER:

2001:923615 HCAPLUS

DOCUMENT NUMBER:

136:37623

TITLE:

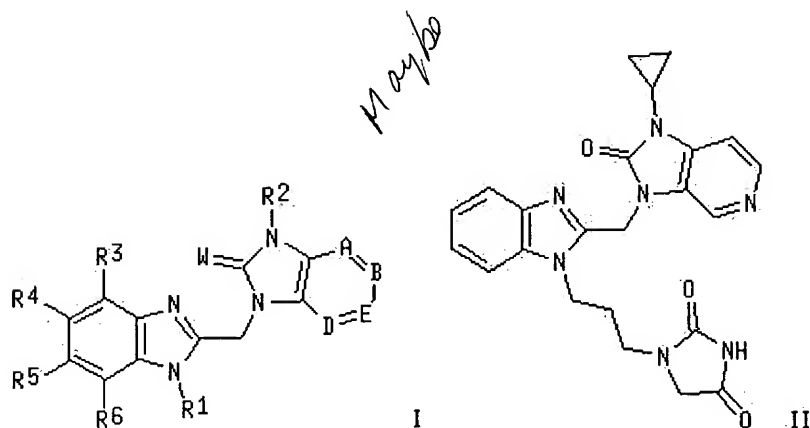
Preparation of imidazopyridine and imidazopyrimidine antiviral agents

INVENTOR(S):

Yu, Kuo-Long; Civiello, Rita L.; Combrink, Keith D.; Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong;

Meanwell, Nicholas A.; Venables, Brian Lee  
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
 SOURCE: PCT Int. Appl., 196 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001095910	A1	20011220	WO 2001-US14775	20010508
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002016309	A1	20020207	US 2001-840279	20010423
US 6489338	B2	20021203		
BR 2001011569	A	20030429	BR 2001-11569	20010508
EP 1311268	A1	20030521	EP 2001-952114	20010508
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004503501	T2	20040205	JP 2002-510088	20010508
NO 2002005977	A	20030129	NO 2002-5977	20021212
PRIORITY APPLN. INFO.:			US 2000-211447P	P 20000613
			US 2001-263363P	P 20010122
			WO 2001-US14775	W 20010508
OTHER SOURCE(S):			MARPAT 136:37623	
GI				



AB The title compds. [I; W = O, S; R1 = (CR'R'')<sub>n</sub>X; X = H, alkyl, cycloalkyl, etc.; n = 2-6; R2 = H, alkyl, cycloalkyl, etc.; R3-R6 = H, halo, alkyl, etc.; A, B, E, D = CH, CQ, N, NO; provided at least one of A, B, E or D is not CH or CQ; Q = halo, alkyl, alkyl substituted with 1-3 halogen atoms; R', R'' = H, alkyl, cycloalkyl, etc.], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. Thus, reacting I [W = O; R1 = (CH<sub>2</sub>)<sub>3</sub>NH<sub>2</sub>; R2 = cyclopropyl; R3-R6 = H; E = N; A, B, D = CH] (prepn. given) with N-chloroacetylurethane in the presence of Na<sub>2</sub>CO<sub>3</sub> in MeCN afforded 39%

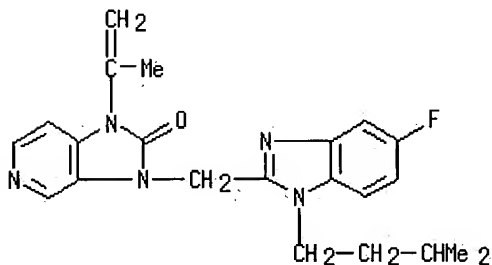
II.TFA. The compds. I showed antiviral activity against RSV with EC50's between 50  $\mu$ M and 0.001  $\mu$ M vs. Ribavirin with an EC50 of 3  $\mu$ M.

IT **380602-42-6P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of imidazopyridine and imidazopyrimidine antiviral agents)

RN 380602-42-6 HCAPLUS

CN 2H-Imidazo[4,5-c]pyridin-2-one, 3-[[5-fluoro-1-(3-methylbutyl)-1H-benzimidazol-2-yl]methyl]-1,3-dihydro-1-(1-methylethenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

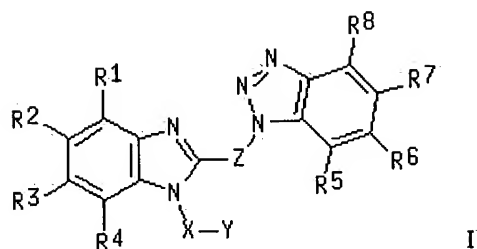
ACCESSION NUMBER: 2000:84617 HCAPLUS  
DOCUMENT NUMBER: 132:122625  
TITLE: Preparation of substituted benzimidazole antiviral agents  
INVENTOR(S): Yu, Kuo-long; Civiello, Rita Lee; Krystal, Mark R.; Kadow, Kathleen F.; Meanwell, Nicholas A.  
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
SOURCE: PCT Int. Appl., 85 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000004900	A1	20000203	WO 1999-US12398	19990720
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2338147	AA	20000203	CA 1999-2338147	19990720
AU 9950809	A1	20000214	AU 1999-50809	19990720
AU 741946	B2	20011213		
EP 1098644	A1	20010516	EP 1999-935302	19990720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

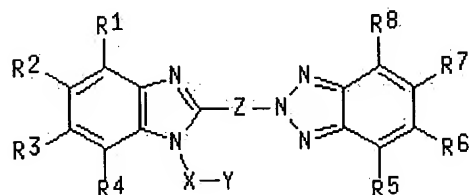


JP 2002521334	T2	20020716	JP 2000-560893	19990720
US 2003139450	A1	20030724	US 2002-289829	20021107
PRIORITY APPLN. INFO.:			US 1998-93387P	P 19980720
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			WO 1999-US12398	W 19990720

OTHER SOURCE(S): MARPAT 132:122625  
GI



I



II

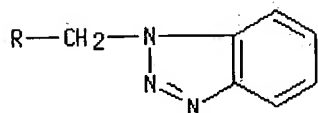
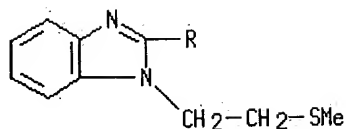
AB The title compds. [I and II; R1-R8 = H, alkyl, NO<sub>2</sub>, etc.; X = straight, branched or cyclic C<sub>2</sub>-12 alkyl, alkenyl, alkynyl; Y = (un)substituted Ph, dioxolane, pyridine, etc.; XY = CH<sub>2</sub>Ph, CH<sub>2</sub>COPh, CH<sub>2</sub>CHOHPh, etc.; Z = (CR<sub>12</sub>R<sub>13</sub>)<sub>n</sub>; n = 1-4; R<sub>12</sub>, R<sub>13</sub> = H, straight, branched or cyclic alkyl], useful in the treatment of viral infections, particularly, for the treatment of respiratory syncytial virus infection, were prepd. Thus, coupling 1-(1H-benzimidazol-2-ylmethyl)-1H-benzotriazole with 2-dimethylaminoethyl chloride hydrochloride in the presence of NaH in THF afforded 23% I [Z = CH<sub>2</sub>; XY = (CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>; R1-R8 = H] which showed 100% HEp-2 cell protection against RSV at 4 µg/mL.

IT **256365-76-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of substituted benzimidazole antiviral agents)

RN **256365-76-1** HCAPLUS

CN 1H-Benzotriazole, 1-[[1-[2-(methylthio)ethyl]-1H-benzimidazol-2-yl]methyl]-  
(9CI) (CA INDEX NAME)



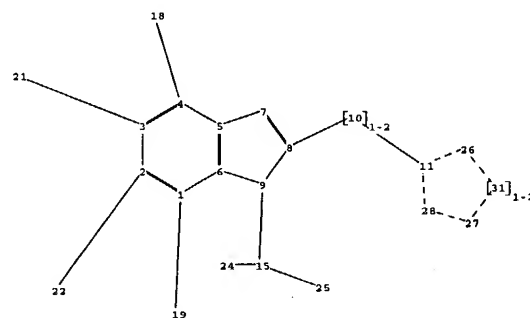
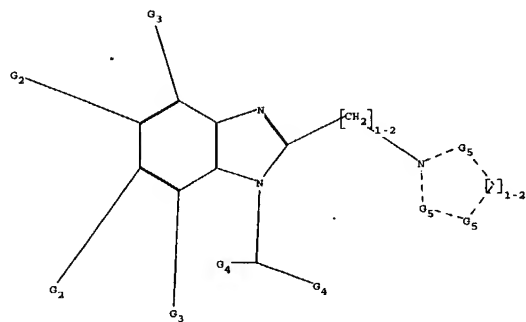
REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

SN 10643411



chain nodes :

10 15 18 19 21 22 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 11 26 27 28 31

chain bonds :

1-19 2-22 3-21 4-18 8-10 9-15 10-11 15-25 15-24

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-26 11-28 26-31 27-28 27-31

exact/norm bonds :

1-19 2-22 3-21 4-18 5-7 7-8 8-9 9-15 11-26 11-28 15-25 15-24 26-31 27-28 27-31

exact bonds :

6-9 8-10 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G2:H,X,Ak

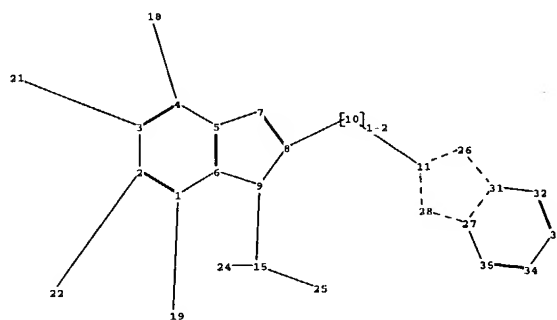
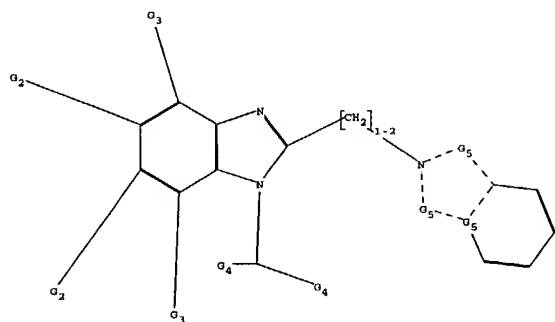
G3:X,H

G4:H,Ak

G5:C,O,N

Match level :

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 15:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom  
 28:Atom 31:Atom



chain nodes :

10 15 18 19 21 22 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 11 26 27 28 31 32 33 34 35

chain bonds :

1-19 2-22 3-21 4-18 8-10 9-15 10-11 15-25 15-24

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-26 11-28 26-31 27-28 27-31 27-35  
31-32 32-33 33-34 34-35

exact/norm bonds :

1-19 2-22 3-21 4-18 5-7 7-8 8-9 9-15 11-26 11-28 15-25 15-24 26-31 27-28  
27-31 27-35 31-32 32-33 33-34 34-35

exact bonds :

6-9 8-10 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G2:H,X,Ak

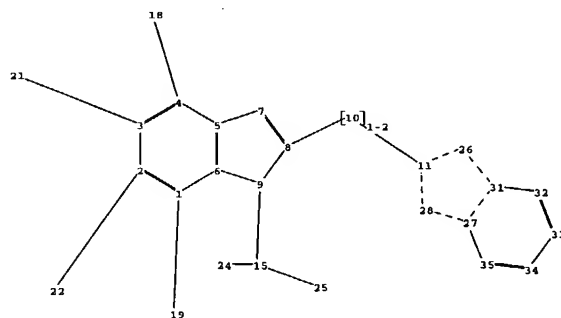
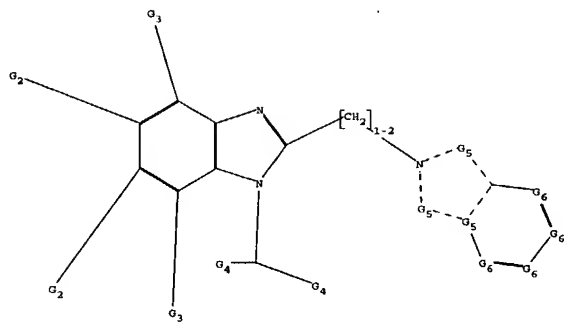
G3:X,H

G4:H,Ak

G5:C,O,N

Match level :

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15:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom  
28:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom



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chain nodes :
  10 15 18 19 21 22 24 25
ring nodes :
  1 2 3 4 5 6 7 8 9 11 26 27 28 31 32 33 34 35
chain bonds :
  1-19 2-22 3-21 4-18 8-10 9-15 10-11 15-25 15-24
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-26 11-28 26-31 27-28 27-31 27-35
  31-32 32-33 33-34 34-35
exact/norm bonds :
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  27-31 27-35 31-32 32-33 33-34 34-35
exact bonds :
  6-9 8-10 10-11
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
  containing 1 :

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G2:H,X,Ak

G3:X,H

G4:H,Ak

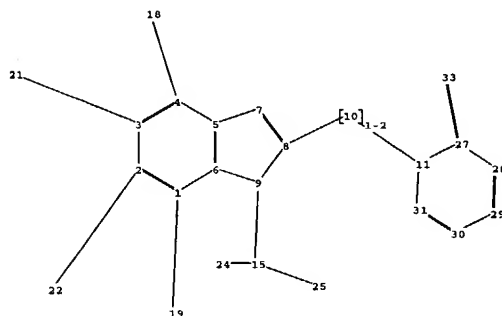
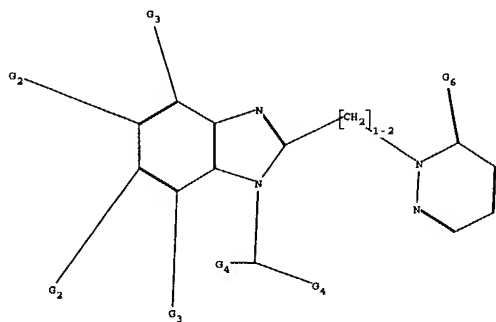
G5:C,O,N

G6:C,N

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Match level :
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  15:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom
  28:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom

```



chain nodes :  
10 15 18 19 21 22 24 25 33  
ring nodes :  
1 2 3 4 5 6 7 8 9 11 27 28 29 30 31  
chain bonds :  
1-19 2-22 3-21 4-18 8-10 9-15 10-11 15-25 15-24 27-33  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-27 11-31 27-28 28-29 29-30 30-31  
exact/norm bonds :  
1-19 2-22 3-21 4-18 5-7 7-8 8-9 9-15 11-27 11-31 15-25 15-24 27-28 27-33  
28-29 29-30 30-31  
exact bonds :  
6-9 8-10 10-11  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G2:H,X,Ak

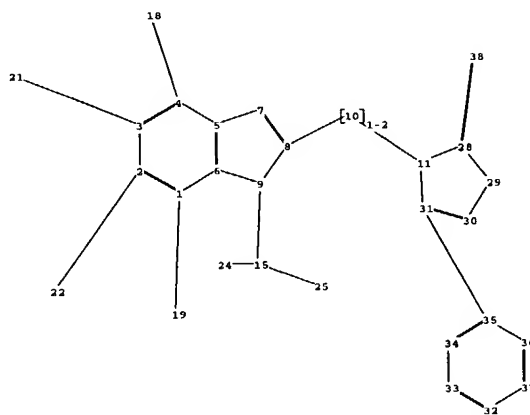
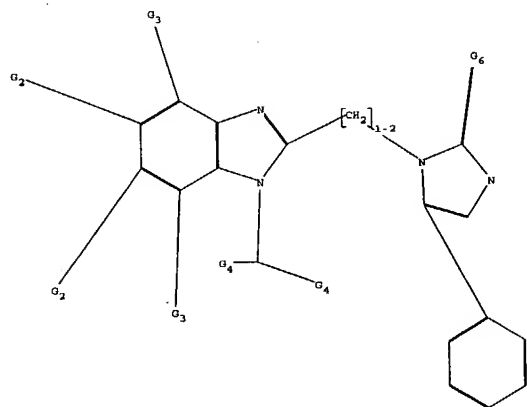
G3:X,H

G4:H,Ak

G5:C,O,N

G6:O,S

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom  
15:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 27:Atom 28:Atom  
29:CLASS 30:Atom 31:Atom 33:CLASS



chain nodes :  
10 15 18 19 21 22 24 25 38  
ring nodes :  
1 2 3 4 5 6 7 8 9 11 28 29 30 31 32 33 34 35 36 37  
chain bonds :  
1-19 2-22 3-21 4-18 8-10 9-15 10-11 15-25 15-24 28-38 31-35  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-28 11-31 28-29 29-30 30-31 32-33  
32-37 33-34 34-35 35-36 36-37  
exact/norm bonds :  
1-19 2-22 3-21 4-18 5-7 7-8 8-9 9-15 11-28 11-31 15-25 15-24 28-29 28-38  
29-30  
exact bonds :  
6-9 8-10 10-11 30-31 31-35  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 32-33 32-37 33-34 34-35 35-36 36-37  
isolated ring systems :  
containing 1 : 11 : 32 :

G2:H,X,Ak

G3:X,H

G4:H,Ak

G5:C,O,N

G6:O,S

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom  
15:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 28:Atom 29:Atom  
30:Atom 31:Atom 32:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS